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Ling Ma
Noel J. Walkington
Carnegie Mellon University

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On Algorithms for Non–Convex Optimization

Ling Ma and Noel J. Walkington*

Abstract. A simple algorithm for the computation of local minima of non–convex problems in one dimension is proposed. This algorithm avoids certain well known local minima which are distant from the global minimum, and can be used to improve the minima obtained using classical descent methods. The calculated minima have mesh scale oscillations typical of weakly converging sequences. It is shown that these local minima converge weakly to the correct limit for certain simple problems; however, numerical evidence suggests that the gradients may not converge to the correct weak limits, and this is verified using asymptotic expansions. Extensions to multiple dimensions and some numerical examples in two dimensions are considered.

1. Introduction. The fundamental idea in the method of calculus of variations is to minimize an energy functional. Since many physical systems take on a configuration which minimizes a natural energy, and since variational techniques have been remarkably successful in predicting the behavior of such systems, this area has a rich history. The variational characterization of such problems also leads to natural numerical schemes for approximating their solution. Typically the solution of the continuous problem lies in a separable Banach space. The problem is then discretized by constructing a finite dimensional subspace, and minimizing over this subspace; a chore suitable for digital computers. Classical problems in the areas of solid mechanics, fluid mechanics, dynamics etc. all have sufficient convexity of the energy to guarantee the existence of well behaved solutions. In this situation, it is easy to construct algorithms that will find the discrete minimizers, and approximation theory establishes how well the discrete solutions approximate the original problem.

It has been known for a long time that if certain convexity assumptions were not satisfied, then there may be no solution (minimizer) of the variational problem. The fundamental work of Young [16] develops a theory of generalized solutions to these problems. At that time, generalized solutions were used mainly in the context of control theory (chattering controls), and not in the context of mechanics. Recently it has been recognized that the generalized solutions developed by Young provided a beautiful characterization of certain fine scale microstructures observed in crystalline materials (metals) [3, 10]. This realization rendered the study of certain microscopic phenomena mathematically tractable, casting it into a variational framework. In principle, the numerical technique outlined above can now be used to approximate the behavior and fine scale phenomena these materials exhibit. However, the generalized solutions are no longer real valued functions, typically they consist of a pair, a function and a parameterized measure. Since such solutions still lie in a separable Banach space, one can, in principle, approximate them using finite dimensional subspaces. This is the approach proposed by Nicolaides and Walkington [15], and requires approximating measures. The parameterized measures that arise in these problems are obtained by taking certain weak limits of a sequences of functions. This leads to an al-

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ternative class of algorithms that only involve real valued functions. The basic idea is to observe that a finite dimensional "approximation" of the original variational problem will still have a solution even when there is no convexity of the energy. By letting the dimension of the subspace go to infinity, one obtains a sequence of functions from which the generalized solution may be deduced. This is the approach taken by Collins and Luskin [8, 7], and Luskin and Ma [13, 14], and it is the practical considerations of this algorithm that we discuss below.

One of the major obstacles to computing with either of the above algorithms is the need to minimize a non–convex function over a finite dimensional space. Simple examples quickly show that the standard minimization algorithms (relaxation, conjugate gradient etc.) fail in this task. Indeed, given a candidate for a solution there is no easy way to decide if it is the minimizer or even close to it. One guide that is implicitly used in [8, 7, 13] is a priori knowledge of the behavior of the generalized solution or microscopic phenomena being modeled. For the model problems calculated in [8, 7, 13] it is known that the discrete solutions should oscillate, and frequently it is known what certain weak limits should be, so the solutions should oscillate about these known limits. Below we present an algorithm for a class of one dimensional variational problems that produces highly oscillatory discrete solutions, and converges to the correct weak limit[1]. While this is a considerable improvement over traditional minimization algorithms, it is possible to show that the sequence of discrete solutions may not converge to the correct generalized solution. This illustrates that the practical solution of these non–convex problems poses subtleties hitherto unsuspected. Indeed, the results of Collins et. al. [6, 5] show that if the global discrete minima could be calculated, the correct generalized solution would result.

In section 2 we propose an algorithm for the calculation of local minimizers, and in section 3 we present some numerical experiments which exhibit the mesh scale oscillations produced by our algorithm. Detailed examination of numerical examples like those of section 3 raised questions about the convergence to the correct generalized solution, and this motivated the asymptotic analysis in section 4 which answers these questions. In section 5 we discuss generalizations to multiple dimensions, and present some numerical examples.

2. An Algorithm for Local Minima. We consider variational problems of the form: minimize

$$I(u) = \int_0^1 F(u') + \frac{1}{2}(u - f)^2, \qquad u \in \mathcal{A},$$

where $\mathcal{A} = \{u \in W^{1,p}(0,1) \mid u(0) = u_0, u(1) = u_R\}$, is the space of admissible functions with boundary conditions prescribed. We assume that $F : \Re \to \Re$ satisfies $cs^p - 1 \leq F(s) \leq Cs^p$, $(c, C > 0)$, and $f : [0,1] \to \Re$ is continuous. This problem is approximated by constructing a uniform mesh on $[0,1]$ with mesh size $h = 1/N$ and minimizing

$$I_h(u) \;=\; \sum_{j=0}^{N-1} hF(u_j') + \frac{1}{2}\sum_{j=1}^{N-1} h(u_j - f_j)^2$$

[1] A discrete solution in the above context is a local minima to the discrete problem.

$$= \sum_{j=0}^{N-1} hF(\frac{u_{j+1}-u_j}{h}) + \frac{1}{2}\sum_{j=1}^{N-1} h(u_j - f_j)^2,$$

over the space of piecewise linear functions on the mesh satisfying the boundary conditions. In the above u_j' is the derivative on the j^{th} interval, and u_j and f_j are the values of u and f at the j^{th} node. The Euler Lagrange equation for the discrete system is

$$(1) \qquad F'(u_{j-1}') - F'(u_j') + h(u_j - f_j) = 0, \qquad j = 1, 2, \ldots, N-1.$$

To motivate our ideas, we consider Young's problem where

$$(2) \qquad F(s) = \frac{1}{4}(s^2-1)^2, \qquad f(x) = 0, \qquad u_0 = u_R = 0,$$

and recall that the continuous variational problem has no solution, while the discrete variational problem does. The continuous problem may have $W^{1,\infty}$ stable local minimizers, but not L^∞ stable local minimizers [2]. That is, there are u and $\epsilon > 0$ such that u minimizes I over $\mathcal{A} \cap B_\epsilon(u; W^{1,\infty})$, where $B_\epsilon(u, W^{1;\infty})$ is the ball in $W^{1,\infty}$ centered at u of radius ϵ. The well known hat functions shown in figure 1 are typical of such local minima. However, there are no functions u that minimize I in $\mathcal{A} \cap B_\epsilon(u; L^\infty)$. Numerical experiments reveal that essentially all classical minimization algorithms will terminate in one of the $W^{1,\infty}$ stable local minima, which may be far from the global minima.

One of the reasons classical algorithms fail is due to a scaling problem. F is a degree four polynomial with argument $(u_{j+1}-u_j)/h$. When h is small, small perturbations of u_j will cause very large variations in $F(u_j')$, swamping the low order term. However, it is the low order term that distinguishes a local minima from a global minima. These ideas motivated the following elementary move:

- For $j = 1, 2, \ldots, N-1$
  - Let $\tilde{u}_j = u_{j+1} + u_{j-1} - u_j$.
  - If $(\tilde{u}_j - f_j)^2 < (u_j - f_j)^2$ replace u_j by $\tilde{u}_j$.

The key point is that, on a uniform mesh, replacing u_j by $\tilde{u}_j$ does not change the energy of the principle part, i.e.

$$F(\frac{u_j - u_{j-1}}{h}) + F(\frac{u_{j+1}-u_j}{h}) = F(\frac{\tilde{u}_j - u_{j-1}}{h}) + F(\frac{u_{j+1}-\tilde{u}_j}{h}).$$

This follows by observing that the above choice of $\tilde{u}_j$ simply interchanges the values of the slope in the two elements adjacent to the j^{th} node. In this circumstance, it is the low order term which determines the outcome of the move. Moreover, this move will not be small in $W^{1,\infty}$; indeed, generically it will change a local maximum to a local minimum. Discrete maximum principles can be established for this algorithm.

LEMMA 2.1. *Let u be a local minima of I_h calculated so that the move above does not lower the energy. If u_j is a strict interior maximum and $u_j - f_j \geq 0$, then either $u_{j-1} - f_j \leq 0$ or, $u_{j+1} - f_j \leq 0$. Similarly, if u_j is a strict interior minima and $u_j - f_j \leq 0$, then either $u_{j-1} - f_j \geq 0$ or $u_{j+1} - f_j \geq 0$.*

Proof. We argue by contradiction. Suppose not, then both $u_{j+1} - f_j$ and $u_{j-1} - f_j$ are greater than 0.

$$\begin{aligned} \tilde{u}_j - f_j &= u_{j-1} + u_{j+1} - u_j - f_j \\ &= (u_{j-1} - f_j) + (u_{j+1} - f_j) - (u_j - f_j) \\ &> -|u_j - f_j|. \end{aligned}$$

It follows that $\tilde{u}_j - f_j \geq u_j - f_j$, otherwise the energy would be lowered by replacing u_j with $\tilde{u}_j$. Then

$$\tilde{u}_j \geq u_j \Rightarrow u_{j+1} + u_{j-1} - u_j \geq u_j \Rightarrow u_{j+1} + u_{j-1} - 2u_j \geq 0,$$

and this contradicts u_j being a strict maximum. □

COROLLARY 2.2. *Let u be a local minima of I_h calculated so that the move above does not lower the energy. Then $\max_j u_j \leq \max(u_0, u_N, \max_j f_j + Ch^{(p-1)/p})$, where C depends upon the energy $I_h(u)$.*

Proof. The lemma shows that at a maxima either $u_j < f_j$ or one of the neighboring points is $\leq f_j$. The coercivity condition on F implies a bound on the $W^{1,p}(0,1)$ norm of the solution, with the bound depending upon $I_h(u)$. It follows that $u \in C^{0,(p-1)/p}$, so that $u_j \leq f_j + u_j - u_{j\pm 1} \leq f_j + Ch^{(p-1)/p}$. □

When f is linear, a minor modification of the proofs above give.

LEMMA 2.3. *Let f be linear, and u be a local minimum of I_h calculated so that the move above does not lower the energy. If $\{u_i - f_i\}_{i=0}^N$ attains a positive strict maximum at j, $1 \leq j \leq N-1$, then either $u_{j-1} - f_{j-1} \leq 0$ or, $u_{j+1} - f_{j+1} \leq 0$. Similarly, if $u_j - f_j \leq 0$ is a strict negative minimum, $1 \leq j \leq N-1$, then either $u_{j-1} - f_{j-1} \geq 0$ or $u_{j+1} - f_{j+1} \geq 0$.*

COROLLARY 2.4. *Let f be linear and u be a local minima of I_h calculated so that the move above does not lower the energy. Then $\max_j (u_j - f_j) \leq \max(u_0 - f_0, u_N - f_N, Ch^{(p-1)/p})$, and $\min_j (u_j - f_j) \geq \min(u_0 - f_0, u_N - f_N, -Ch^{(p-1)/p})$.*

When f is linear and $u_0 = f(0)$ and $u_N = f(1)$ the generalized solution to the non-homogeneous Young problem is $u = f$. This immediately leads to an L^∞ rate of convergence for our algorithm.

THEOREM 2.5. *Let f be linear, and $\{u_h\}_{h>0}$, $u_h(0) = f(0)$, $u_h(1) = f(1)$, be a sequence of local minima for the discrete non-homogeneous Young problem calculated so that the move above does not lower the energy. Moreover, assume that the energies $I_h(u_h)$ are bounded. Then $\|u_h - f\|_{L^\infty(0,1)} \leq Ch^{(p-1)/p}$.*

In practice it is easy to guarantee that the energies $I_h(u_h)$ are bounded. One simply chooses the same initial guess for u_h independently of h.

Knowing that the solutions converge to the correct weak limit, it is natural to ask if the energy converges to the infimum, and if the Young measure generated by the gradients corresponds to the generalized solution of the continuous variational problem. Both of these questions can be answered negatively. We first present some numerical experiments which suggest a negative answer. The numerical solutions are all of a particular form which motivates asymptotic expansions substantiating the trends observed. However, note that the numerical examples do have mesh scale oscillations about the correct weak limit, so could easily be mistaken for a minimizing sequence of the continuous problem.

3. Numerical Examples. We present several numerical examples which illustrate the operation of our algorithm. We will consider Young's problem where F and f are as in (1), and a non–homogeneous version where $f(x) = 0.2x$, $u(0) = f(0)$, and $u(1) = f(1)$. In all examples the initial guess for u was $u(x) = f(x) + \sin(\pi x)$, and the following elementary algorithm was used to locate a local minima.

- Set $\epsilon > 0$.
- For $j = 1, 2, \ldots, N-1$
  - Replace u_j by $u_j + \epsilon$ if this lowers the energy.
  - Replace u_j by $u_j - \epsilon$ if this lowers the energy.

We started with $\epsilon = 1$ and alternated this update with the move given previously. When the process stopped ϵ was halved and the process repeated until ϵ was negligible (typically $\epsilon = 10^{-11}$). This algorithm is very robust and, unlike descent methods based upon the derivative, may not get stuck in saddle points.

Figure 2 show plots of the solutions obtained for Young's problem when $N = 64$, 127 and 128. Note that they all exhibit mesh scale oscillations and there are two very distinct patterns that emerge. When the number of nodes is even, it is possible for the solution to oscillate as shown in figure 2a ($N = 64$). Clearly this pattern is not possible for an odd number of nodes, and in this instance the pattern shown in figure 2b emerges. However, it was observed that the latter pattern was more "stable" for N big, since meshes with an even number of nodes would decouple into groups of odd nodes where the odd nodded pattern would appear, as shown in figure 2c where the solution for a mesh on $N = 128$ grid points decoupled into two odd solutions consisting of 63 and 65 nodes.

Solutions for the non–homogeneous problem are given in figure 3 for $N = 64$, 128, and 256. These solutions all consist of oscillation packets, each packet being very similar and each having an odd number of nodes. While it is not clear from the plots, the gradients of the oscillations do not get closer to ± 1 as N increases. Moreover, the energy, given if figure 6, sometimes increased as the mesh was refined.

4. Asymptotic Estimates. When f is linear, our numerical experiments motivate the following asymptotic expansion for the numerical solution u,

$$\begin{aligned} u_{2j} &= 2jh\alpha + h(\nu_{2j} + h\tilde{\nu}_{2j} + \ldots), \\ u_{2j+1} &= (2j+1)h\alpha + h(\beta + \nu_{2j+1} + h\tilde{\nu}_{2j+1} + \ldots), \end{aligned}$$

where $\alpha = f'$ is constant. The boundary condition $u(0) = f(0)$ requires $0 = \nu_0 = \tilde{\nu}_0 = \ldots$, and the right hand boundary condition $u_N = f(1)$ requires $0 = \nu_N = \tilde{\nu}_N = \ldots$ if N is even, and $\nu_N = -\beta$, $0 = \tilde{\nu}_N = \ldots$ when N is odd.

The derivatives of the piecewise linear function u then become

$$\begin{aligned} u'_{2j} &= \alpha + \beta + (\nu_{2j+1} - \nu_{2j}) + h(\tilde{\nu}_{2j+1} - \tilde{\nu}_{2j}) + \ldots \\ u'_{2j+1} &= \alpha - \beta + (\nu_{2j+2} - \nu_{2j+1}) + h(\tilde{\nu}_{2j+2} - \tilde{\nu}_{2j+1}) + \ldots \end{aligned}$$

so that

$$\begin{aligned} F'(u'_{2j}) = {} & F'(\alpha+\beta) + F''(\alpha+\beta)[\nu_{2j+1} - \nu_{2j} + h(\tilde{\nu}_{2j+1} - \tilde{\nu}_{2j})] + \\ & \frac{1}{2}F'''(\alpha+\beta)(\nu_{2j+1} - \nu_{2j})^2 + \ldots \end{aligned}$$

$$F'(u'_{2j+1}) = F'(\alpha-\beta) + F''(\alpha-\beta)[\nu_{2j+2} - \nu_{2j+1} + h(\tilde{\nu}_{2j+2} - \tilde{\nu}_{2j+1})] + \frac{1}{2}F'''(\alpha-\beta)(\nu_{2j+2} - \nu_{2j+1})^2 + \ldots$$

In order for the expansion for u to be meaningful, we look for bounded values of ν and $\tilde{\nu}$. Similarly, in order for the expansion for the derivative u' to be meaningful, we require $\nu_{j+1} - \nu_j$, $\tilde{\nu}_{j+1} - \tilde{\nu}_j$ etc. to be of order h. The solutions we obtain below satisfy these assumptions; indeed, ν and $\tilde{\nu}$ consist of a smooth piece plus a small oscillatory component of size $O(h^2)$.

Substituting the above into the discrete Euler Lagrange equation (1) gives

$$F'(\alpha-(-1)^j\beta) - F'(\alpha+(-1)^j\beta) +$$
$$\left[F''(\alpha-(-1)^j\beta)(\nu_j - \nu_{j-1}) - F''(\alpha+(-1)^j\beta)(\nu_{j+1} - \nu_j)\right] +$$
$$\left[F''(\alpha-(-1)^j\beta)(\tilde{\nu}_j - \tilde{\nu}_{j-1})h - F''(\alpha+(-1)^j\beta)(\tilde{\nu}_{j+1} - \tilde{\nu}_j)h\right.$$
$$\left.+\frac{1}{2}F'''(\alpha-(-1)^j\beta)(\nu_j - \nu_{j-1})^2 - \frac{1}{2}F'''(\alpha+(-1)^j\beta)(\nu_{j+1} - \nu_j)^2\right] + \ldots$$
$$h^2(\nu_j + h\tilde{\nu}_j + \ldots) = h^2 \begin{cases} 0 & j \ even \\ -\beta & j \ odd \end{cases}$$

We now equate terms that are (formally) of similar size. The correct groupings are most easily recognized when β is zero, since then it is clear that the terms associated with F'' are discretizations of the second derivative.

$$F'(\alpha+\beta) = F'(\alpha-\beta),$$

and for $j = 1, 2, \ldots, N-1$,

$$F''(\alpha-(-1)^j\beta)(\nu_j - \nu_{j-1}) - F''(\alpha+(-1)^j\beta)(\nu_{j+1} - \nu_j) + h^2\nu_j = h^2 \begin{cases} 0 & j \ even, \\ -\beta & j \ odd, \end{cases}$$

$$F''(\alpha-(-1)^j\beta)(\tilde{\nu}_j - \tilde{\nu}_{j-1}) - F''(\alpha+(-1)^j\beta)(\tilde{\nu}_{j+1} - \tilde{\nu}_j) + h^2\tilde{\nu}_j$$
$$= \frac{-1}{2h}\left[F'''(\alpha-(-1)^j\beta)(\nu_j - \nu_{j-1})^2 - F'''(\alpha+(-1)^j\beta)(\nu_{j+1} - \nu_j)^2\right].$$

Writing

$$a_{j+1/2} = F''(\alpha+(-1)^j\beta),$$

the latter equations become

$$a_{j-1/2}(\nu_j - \nu_{j-1}) - a_{j+1/2}(\nu_{j+1} - \nu_j) + h^2\nu_j = h^2 \begin{cases} 0 & j \ even, \\ -\beta & j \ odd, \end{cases}$$

$$a_{j-1/2}(\tilde{\nu}_j - \tilde{\nu}_{j-1}) - a_{j+1/2}(\tilde{\nu}_{j+1} - \tilde{\nu}_j) + h^2\tilde{\nu}_j$$
$$= \frac{-1}{2h}\left[F'''(\alpha-(-1)^j\beta)(\nu_j - \nu_{j-1})^2 - F'''(\alpha+(-1)^j\beta)(\nu_{j+1} - \nu_j)^2\right].$$

We introduce the following discrete norms.

$$\|\nu\|_{\ell^2}^2 = \sum_{j=1}^{N-1} h\nu_j^2, \qquad \|\nu\|_{\ell^\infty} = \max_{1\le j\le N-1} |\nu_j|,$$

$$\|\nu\|_{h^1}^2 = \sum_{j=0}^{N-1} h a_{j+1/2}\left(\frac{\nu_{j+1}-\nu_j}{h}\right)^2, \qquad \|\nu\|_{w^{1,\infty}} = \max_{1\le j\le N} a_{j-1/2}\frac{|\nu_j-\nu_{j-1}|}{h}.$$

$$\|\nu\|_{h^2}^2 = \sum_{j=1}^{N-1} h\left(\frac{a_{j+1/2}(\nu_{j+1}-\nu_j)-a_{j-1/2}(\nu_j-\nu_{j-1})}{h^2}\right)^2,$$

The following lemma is and elementary application of summation by parts.

LEMMA 4.1. *Let the coefficients $a_{j+1/2}$ be non-negative and uniformly bounded. If ν satisfies*

$$a_{j-1/2}(\nu_j-\nu_{j-1}) - a_{j+1/2}(\nu_{j+1}-\nu_j) + h^2\nu_j = h^2 f_j, \qquad \nu_0 = 0,$$

then $\|\nu\|_{\ell^2}$, $\|\nu\|_{h^1}$, $\|\nu\|_{w^{1,\infty}}$, and $\|\nu\|_{h^2}$ are all bounded by a constant $C(\|f\|_{\ell^2}, \nu_N)$ depending only upon $\|f\|_{\ell^2}$ and ν_N.

If $\tilde\nu$ satisfies

$$a_{j-1/2}(\tilde\nu_j-\tilde\nu_{j-1}) - a_{j+1/2}(\tilde\nu_{j+1}-\tilde\nu_j) + h^2\tilde\nu_j = h(g_{j+1/2}-g_{j-1/2}), \qquad \nu_0 = 0,$$

then $\|\tilde\nu\|_{\ell^2}$ and $\|\tilde\nu\|_{h^1}$ are bounded by a constant $C(\|g\|_{\ell^2}, \nu_N)$ depending only upon $\|g\|_{\ell^2}$ and ν_N.

Moreover $\|\nu\|_{\ell^\infty}$ and $\|\tilde\nu\|_{\ell^\infty}$ are bounded by a constants which depend additionally upon $\min_{1\le j\le N} a_{j-1/2}$.

4.1. Calculation of the Energy. Our numerical experiments suggest that the solution consists of one or more packets consisting of $M < N$ node points. Accordingly, we calculate the energy for a typical packet, and afterwards multiply by the number of packets ($N/M = 1/(hM)$).

$$\begin{aligned}
E_M &= \sum_{j=0}^{M-1} hF(u_j') + \frac{1}{2}\sum_{j=1}^{M-1} h(u_j-f_j)^2 \\
&= \sum_{j=0\,\text{odd}}^{M-1} hF[\alpha-\beta+(\nu_{j+1}-\nu_j)+h(\tilde\nu_{j+1}-\tilde\nu_j)+\cdots] \\
&\quad + \sum_{j=0\,\text{even}}^{M-1} hF[\alpha+\beta+(\nu_{j+1}-\nu_j)+h(\tilde\nu_{j+1}-\tilde\nu_j)+\cdots] \\
&\quad + \frac{1}{2}\sum_{j=1\,\text{odd}}^{M-1} h^3(\beta+\nu_j+h\tilde\nu_j+\cdots)^2 + \frac{1}{2}\sum_{j=1\,\text{even}}^{M-1} h^3(\nu_j+h\tilde\nu_j+\cdots)^2 \\
&= \lfloor M/2\rfloor h[F(\alpha-\beta)+h^2\beta^2/2] + \lfloor (M+1)/2\rfloor hF(\alpha+\beta) + F'(\alpha\pm\beta)h\nu_M \\
&\quad + \frac{h}{2}\sum_{j=0}^{M-1}\left[a_{j+1/2}(\nu_{j+1}-\nu_j)^2 + h^2\nu_j^2\right] + \beta h^3\sum_{j=1\,\text{odd}}^{M-1}\nu_j + O(h^3).
\end{aligned}$$

($\lfloor x \rfloor$ denotes the greatest integer less than or equal to x.) The equation for ν reveals that

$$\sum_{j=0}^{M-1} \left[a_{j+1/2}(\nu_{j+1} - \nu_j)^2 + h^2 \nu_j^2 \right] = a_{M-1/2}(\nu_M - \nu_{M-1})\nu_M - \beta h^2 \sum_{j=1 \text{ odd}}^{M-1} \nu_j,$$

giving

$$\begin{aligned} E_M &= \lfloor M/2 \rfloor h[F(\alpha - \beta) + h^2\beta^2/2] + \lfloor (M+1)/2 \rfloor h F(\alpha + \beta) + F'(\alpha \pm \beta) h \nu_M \\ &\quad + \frac{1}{2} h a_{M-1/2}(\nu_M - \nu_{M-1})\nu_M + \frac{1}{2}\beta h^3 \sum_{j=1 \text{ odd}}^{M-1} \nu_j + O(h^3). \end{aligned} \tag{3}$$

Note that the last term is an approximation to the integral of ν,

$$\frac{1}{2}\beta h^3 \sum_{j=1 \text{ odd}}^{M-1} \nu_j = \frac{1}{4}\beta h^2 \int_0^{Mh} \nu + O(h^3).$$

In summary, given a specific right hand boundary condition, the energy can be estimated if the integral of ν and the flux at the right hand end can be estimated. This will be done by solving the continuous problem which ν approximates.

4.2. Young's Problem. In this section we explicitly calculate the asymptotic solution for Young's problem, where F is given as in (2), and show that it is in agreement with the computed results.

For Young's problem, the equation $F'(\alpha + \beta) = F'(\alpha - \beta)$ gives either $\beta = 0$ or

$$\beta = \pm\sqrt{1 - 3\alpha^2},$$

and by symmetry, it suffices to consider the positive root $\beta > 0$. The coefficients of the equation for ν and $\tilde{\nu}$ then become

$$a_{j+1/2} = F''(\alpha + (-1)^j\beta) = 2(1 - 3\alpha^2) + 6(-1)^j\alpha\beta = 2\beta(\beta + 3(-1)^j\alpha).$$

In order for these coefficients to be positive, it is necessary that

$$\alpha^2 < 1/12 \quad \text{or} \quad |\alpha| < 0.289...$$

Finally, note that ν consists of a small oscillating part plus a "smooth" part. To illustrate this, observe that the right hand side of the equation for ν may be written as

$$-\frac{1}{2}\beta + \frac{1}{2}(-1)^j\beta = \begin{cases} 0 & j \text{ even} \\ -\beta & j \text{ odd} \end{cases}$$

We then write $\nu = \nu^{(1)} + \nu^{(2)}$ where $\nu^{(2)}$ is of the form $\nu_h^{(2)} = (-1)^j c$ and satisfies

$$a_{j-1/2}(\nu_j^{(2)} - \nu_{j-1}^{(2)}) - a_{j+1/2}(\nu_{j+1}^{(2)} - \nu_j^{(2)}) + h^2\nu_j^{(2)} = h^2\frac{1}{2}(-1)^j\beta.$$

The constant c can be explicitly evaluated to give

$$\nu^{(2)} = \frac{\beta}{2(8\beta^2 + h^2)}(-1)^j h^2. \tag{4}$$

This portion of the solution is very small, $O(h^2)$; also, its derivative is small, $O(h)$. The calculation of $\nu^{(1)}$ is vastly simplified if f and hence α is zero, so we consider this case separately.

4.2.1. Homogeneous Problem. When $\alpha = 0$, we immediately get $\beta = 1$, $\nu = \nu^{(1)} + \nu^{(2)}$ where

$$\nu^{(2)} = \frac{(-1)^j}{16 + 2h^2} h^2,$$

and $a_{j+1/2} = 2$, so that

$$-\nu_{j-1}^{(1)}) + 2\nu_j^{(1)} - \nu_{j+1}^{(1)} + \frac{1}{2}h^2\nu_j^{(1)} = -\frac{1}{4}h^2.$$

Clearly this is a discretization of

$$-w'' + \frac{1}{2}w = -\frac{1}{4},$$

which has solution

$$w(x) = -\frac{1}{2} + A\cosh(x/\sqrt{2}) + B\sinh(x/\sqrt{2}),$$

where A and B are constants chosen to satisfy boundary conditions. Standard results show that $\nu_j^{(1)}$ is an $O(h^2)$ approximation to $w(jh)$, and the derivatives $(\nu_j^{(1)} - \nu_{j-1}^{(1)})/h$ approximate $w'(jh)$ to $O(h)$. We will approximate $\nu^{(1)}$ by w, and since this introduces errors similar in size to the magnitude of $\nu^{(2)}$, we simply consider w as an approximation to ν.

When N is even, the boundary conditions become $w(0) = w(1) = 0$ so that

$$w(x) = \frac{1}{2}\left(\cosh(x/\sqrt{2}) - 1\right) - \frac{\cosh(1/\sqrt{2}) - 1}{2\sinh(1/\sqrt{2})}\sinh(x/\sqrt{2}),$$

and when N is odd the right hand boundary condition becomes $w(1) = -\beta = -1$, so

$$w(x) = \frac{1}{2}\left(\cosh(x/\sqrt{2}) - 1\right) - \frac{\cosh(1/\sqrt{2}) + 1}{2\sinh(1/\sqrt{2})}\sinh(x/\sqrt{2}).$$

We can now calculate the energy for this problem. Note that $F(\alpha \pm \beta) = F'(\alpha \pm \beta) = 0$ when $\alpha = 0$, $\beta = 1$, so that many of the terms in (3) vanish. When there is a single "packet" as in figures 2a ($N = 64$) and (2b) ($N = 127$), we obtain

$$\begin{aligned} E &= \frac{1}{2}\lfloor N/2 \rfloor h^3\beta^2 + \frac{1}{2}ha_{N-1/2}(\nu_N - \nu_{N-1})\nu_N + \frac{1}{2}\beta h^3 \sum_{j=1\,\text{odd}}^{N-1} \nu_j + O(h^3) \\ &= \frac{1}{4}h^2 + h^2 w'(1)w(1) + + \frac{1}{4}h^2 \int_0^1 w(x)\,dx + O(h^3) \end{aligned}$$

When N is even

$$E = \left(\frac{1}{8} + \frac{\cosh(1/\sqrt{2}) - 1}{2\sqrt{2}\sinh(1/\sqrt{2})}\right) h^2 + O(h^3) \simeq 0.2450395425h^2,$$

and when N is odd

$$E = \left(\frac{1}{8} + \frac{\cosh(1/\sqrt{2}) + 1}{2\sqrt{2}\sinh(1/\sqrt{2})}\right) h^2 + O(h^3) \simeq 1.1663273527h^2.$$

No. Nodes	Numerical Energy	Asymptotic Energy
64	5.98215 E-5	5.98241 E-5
127	7.22980 E-5	7.23124 E-5
128	2.54123 E-4	2.54308 E-4

FIG. 5. *Comparison of asymptotic and numerical energies.*

The final example shown in figure 2 is for $N = 128$. The computed solution for this problem broke into two distinct "packets", each representative of the asymptotic solution with N odd ($M_1 = 63$ and $M_2 = 65$). The energy can be estimated to $O(h^3)$ by $E = E_{63} + E_{65} \simeq 2E_{64}$ provided we use the boundary conditions appropriate to an odd number of grid points i.e. $w(0) = 0$ and $w(1/2) = -1$, giving

$$E = \left(\frac{1}{8} + \frac{\cosh(1/\sqrt{8}) + 1}{\sqrt{2}\sinh(1/\sqrt{8})}\right) h^2 + O(h^3) \simeq 4.166580118h^2.$$

These calculations enable us to explicitly compare the asymptotic predictions with the numerical results. In figure 4 we plot the computed solution with the leading order term in our expansion subtracted out. Observation of the scale on the y–axis shows that the difference is certainly a factor of h smaller. Figure 5 compares the predicted energy with that calculated; again, there is remarkably close agreement.

These calculations show that, provided our algorithm continues to produce this class of solutions, that the energy will converge to zero. Moreover, the sequence of solutions will also generate the correct Young measure, $(1/2)\delta_{-1} + (1/2)\delta_{+1}$, since $u'_{2j} = 1 + O(h)$ and $u'_{2j+1} = -1 + O(h)$. Note, however, that the correct oscillations are easily accommodated on the mesh. Our next example, $f(x) = 0.2x$ ($\alpha = 0.2$), has a Young measure of $(2/5)\delta_{-1} + (3/5)\delta_{+1}$, and representation of the corresponding oscillations would require at least 5 grid points. In this situation, the solutions given by our algorithm do not have energies going to zero, and the oscillations do not have slopes ± 1.

4.2.2. Non–Homogeneous Problem. When $\alpha \neq 0$ we have $\nu = \nu^{(1)} + \nu^{(2)}$ where $\nu^{(2)}$ is given in (4) and $\nu^{(1)}$ satisfies

$$a_{j-1/2}(\nu_j^{(1)} - \nu_{j-1}^{(1)}) - a_{j+1/2}(\nu_{j+1}^{(1)} - \nu_j^{(1)}) + h^2\nu_j^{(1)} = -h^2\frac{1}{2}\beta, \qquad \nu_0^{(1)} = 0, \quad \nu_M^{(1)} = -\beta,$$

where $a_{j+1/2} = a + (-1)^j b$, $a = 2\beta^2$, $b = 6\alpha\beta$, $\beta = \sqrt{1 - 3\alpha^2}$. Note that all of the numerical examples had oscillation packets consisting of an odd number of nodes, so we consider the corresponding right hand boundary condition.

The equation for $\nu^{(1)}$ resembles the discretization of a continuous problem having a highly oscillatory coefficient. Homogenization theory [4] shows that the solution of such problems can be approximated by the solution of a suitably averaged equation. Discretization of these problems has been considered in [1]; however, for this particular problem direct computations can be used to verify that if w is the solution of

$$\bar{a}(w_j - w_{j-1}) - \bar{a}(w_{j+1} - w_j) + h^2 w_j = -h^2\frac{1}{2}\beta, \qquad w_0 = 0, \quad w_M = -\beta,$$

then w approximates $\nu^{(1)}$ when

$$\frac{1}{\bar{a}} = \frac{1}{2}\left(\frac{1}{a+b} + \frac{1}{a-b}\right) = \frac{a}{a^2-b^2} = \frac{1}{2}\frac{1}{(1-12\alpha^2)}.$$

In particular $\|w-\nu^{(1)}\|_{\ell^\infty} \le C/M$, and if the fluxes are defined by $V_{j+1/2} = a_{j+1/2}(\nu^{(1)}_{j+1} - \nu^{(1)}_j)/h$, and $W_{j+1/2} = \bar{a}(w_{j+1}-w_j)/h$, then $\|W-V\|_{\ell^\infty} \le C/M$. The problem for w is clearly a second order discretization of

$$-\bar{a}w'' + w = -\beta/2, \qquad w(0) = 0, \quad w(Mh) = -\beta,$$

so that $\nu^{(1)}$ and hence ν can be approximated to $O(1/M)$ by the solution of the continuous problem

$$w(x) = \frac{\beta}{2}\left(\cosh(x/\sqrt{\bar{a}}) - 1\right) - \frac{\beta}{2}\frac{\cosh(Mh/\sqrt{\bar{a}})+1}{\sinh(Mh/\sqrt{\bar{a}})}\sinh(x/\sqrt{\bar{a}}).$$

The energy for an oscillation packet of M nodes becomes

$$\begin{aligned} E_M &= \frac{1}{2}\left[(M-1)F(\alpha-\beta) + (M+1)F(\alpha+\beta)\right]h - F'(\alpha\pm\beta)\beta h + \\ &\quad \frac{1}{2}\left[\frac{1}{2}(M-1)\beta h - \bar{a}w'(Mh) + \frac{1}{2}\int_0^{Mh} w\right]\beta h^2 + O(h^2/M) \\ &= \frac{1}{2}\left[(M-1)F(\alpha-\beta) + (M+1)F(\alpha+\beta)\right]h - F'(\alpha\pm\beta)\beta h + \\ &\quad \frac{1}{4}\left[\frac{1}{2}Mh + \sqrt{\bar{a}}\frac{\cosh(Mh/\sqrt{\bar{a}})+1}{\sinh(Mh/\sqrt{\bar{a}})}\right]\beta^2h^2 + O(h^2/M) \end{aligned}$$

For the energy function F given in (2) this reduces to

$$E_M = \alpha^2(1-2\alpha^2)Mh - 2\alpha\beta^3 h + \frac{1}{4}\left[\frac{1}{2}Mh + \sqrt{\bar{a}}\,\frac{\cosh(Mh/\sqrt{\bar{a}})+1}{\sinh(Mh/\sqrt{\bar{a}})}\right]\beta^2h^2 + O(h^2/M)$$

If the solution consists of packets of M oscillations, there will be $1/Mh$ of them, so that the energy becomes

$$E = \alpha^2(1-2\alpha^2) - 2\alpha\beta^3/M + \frac{1}{4}\left[\frac{1}{2} + \sqrt{\bar{a}}\,\frac{\cosh(Mh/\sqrt{\bar{a}})+1}{Mh\sinh(Mh/\sqrt{\bar{a}})}\right]\beta^2h^2 + O(h/M^2).$$

In computed examples, the oscillation packets varied slightly in size, so in principle one should add up the energies corresponding to each of the different M's encountered. Since counting oscillations is tedious for the finer meshes, we simply counted the number of wave packets (which did not seem to grow without bound) and set $M = 1/Kh$ into the above, where K is the number of packets. Figure 6 compares the energy computed this way with that of the computed solution.

Again, the asymptotic energies agree with the computed values sufficiently closely to verify the validity of our expansion. Moreover, it is clear that as $h \to 0$ and $M \to \infty$ that the energy converges to $E \to \alpha^2(1-2\alpha^2) \neq 0$ (0.0368 when $\alpha = 0.2$), and $u'_{2j} \to \alpha+\beta$ (1.1381), $u'_{2j+1} \to \alpha-\beta$ (−0.7381), giving $\nu = (1/2)\delta_{\alpha+\beta} + (1/2)\delta_{\alpha-\beta} \neq (3/5)\delta_{+1} + (2/5)\delta_{-1}$.

No. Nodes	No. Packets	Numerical Energy	Asymptotic Energy
64	6	0.0111796	0.0099009
127	9	0.0162671	0.0157068
128	6	0.0225006	0.0223360
256	12	0.0224935	0.0223293
512	12	0.0293334	0.0293127

FIG. 6. *Comparison of asymptotic and numerical energies.*

5. Multi Dimensional Problems. While it is clear that the one dimensional examples with their undesirable behavior can be extended to two or more dimensions, this was not our original goal. The original intent was to find algorithms that would find "better" local minima than traditional descent methods. In particular, we wanted algorithms that would develop the fine scale oscillations that must be present in any minimizing sequence. Given that this was accomplished in one dimension with a very simple move, it is natural to ask if similar moves exist for problems in multiple dimensions. In this section we show that such moves can be defined; however, examples will show that they are not as successful at producing fine scale oscillations as in one dimension.

For definiteness, we consider the scalar problem in two dimensions from [5].

$$I(u) = \int_\Omega F(\nabla u) + f(u), \qquad u \in W_0^{1,4}(\Omega),$$

where

$$F(\nabla u) = |\nabla u - \mathbf{w}_1|^2 |\nabla u - \mathbf{w}_2|^2, \qquad f(u) = \frac{1}{2}u^2.$$

$\mathbf{w}_1$ and $\mathbf{w}_2 \in \Re^2$ are the wells where F vanishes.

Analogous with the one dimensional problem we discretize this problem by considering piecewise linear functions constructed on a triangulation $\mathcal{T}_h$ of Ω to get

$$I_h(u) = \sum_{T \in \mathcal{T}_h} |T| F(\nabla u|_T) + \sum_{j \in \mathcal{N}_h} |A_j| f(u_j),$$

where $\mathcal{N}_h$ is the set of nodes in the triangulation, and A_j is the (complementary) area associated with node j.

The idea of the one dimensional problem was to change a nodal value, $u_j \mapsto \tilde{u}_j$, so that the principle part of the energy did not change. The low order term then determines if the move was accepted. Note that if we consider the principle part of the energy for the two dimensional problem as a function of u_j only (with all other nodal values fixed),

$$p(u_j) = \sum_{T \in \mathcal{T}_h} |T| F(\nabla u|_T),$$

then p is a polynomial of degree four. We may then seek $\tilde{u}_j$ such that $p(\tilde{u}_j) = p(u_j)$. Since $p(\tilde{u}_j) - p(u_j)/(\tilde{u}_j - u_j)$ is a polynomial of degree three, it will always have a real root, implying the existence of $\tilde{u}_j$ typically distinct from u_j.

The results using this algorithm are mixed in the sense that sometimes it produces fine scale oscillation and sometimes it doesn't make any difference. Indeed it may even slow down the convergence of the descent method to a local minimum. In all of the examples below, we used the simple stepping algorithm presented in Section 3 alternated with the move above. We considered $\Omega = (0,1)^2$, and triangular meshes were made by dividing a uniform square mesh along the diagonals with slope -1. The initial guess was always taken to be $u(x,y) = \sin(\pi x)\sin(\pi y)$. Computations were made with $\mathbf{w}_1 = (-1,-1)$, $\mathbf{w}_2 = (1,1)$ and $\mathbf{w}_1 = (-1,1)$, $\mathbf{w}_2 = (1,-1)$. The former will produce oscillations whose contours are along a diagonal of slope -1 so are easily represented on the mesh, the latter has oscillations with contours having slope $+1$, so the mesh will not interpolate such oscillations well. All of the pictorial results are shown using a gray scale, with one well colored white and the other black, and the gray scale indicating how close the gradient is to one of the wells. The principle part of the energy will then be small in the purely white or black regions, and gray will indicate higher energy.

Figures 7a, and 8a show the solution obtained using the descent algorithm alone. Clearly the solutions sort themselves into the coarse oscillations with period $O(h^{1/2})$ observed in [5]. Aside from interpolation limitations imposed by the mesh, the solutions are very similar. Figures 7b and 8b show the solutions obtained when the move above was alternated with the descent iterations. Alignment of the mesh with the contours of the oscillations results in mesh scale oscillations with a few imperfections where different microstructures meet. Moreover, the composite algorithm converged much faster to the local minimum. When the mesh is not aligned with the contours of the oscillations, there was no change in the solution; moreover, alternating with the extra move slowed the convergence. These mesh dependent problems are a serious limitation of this approach (see also [11]). We also note that changing the initial guess to $u \equiv 0$ results in the almost perfect microstructure shown in figure 9 when the contours are aligned with the mesh.

One problem that could be anticipated with above move is depicted in figure 10. Suppose that the mesh was exactly aligned with the microstructure; however, at a particular stage the oscillations are too coarse, as in figure 7a. Then raising or lowering one node can not result in a finer band of oscillations, since a situation similar to that shown in figure 10a will result, where some of the elements will have gradients distant from both wells. This problem is not so predominant with the Crouzeix–Raviart non–conforming elements that have recently been proposed for this class of problems [9, 12]. Recall that these are piecewise linear triangular elements that are continuous only at the mid sides of the elements. Figure 10b shows that adjusting one nodal value of these elements may simply increase the scale of oscillation.

Figures 11 and 12 are the analogue of figure 7 and 8 with non–conforming elements. The qualitative behavior for the descent algorithm alone is similar to that of the conforming elements. However, when the contours are aligned with the mesh, the composite algorithm gives almost perfect mesh scale oscillations, while it results in a garbled solution when the contours are not aligned with the mesh. One other problem with this element is that it is difficult to determine from the plots in what direction the oscillations are supposed to be aligned.

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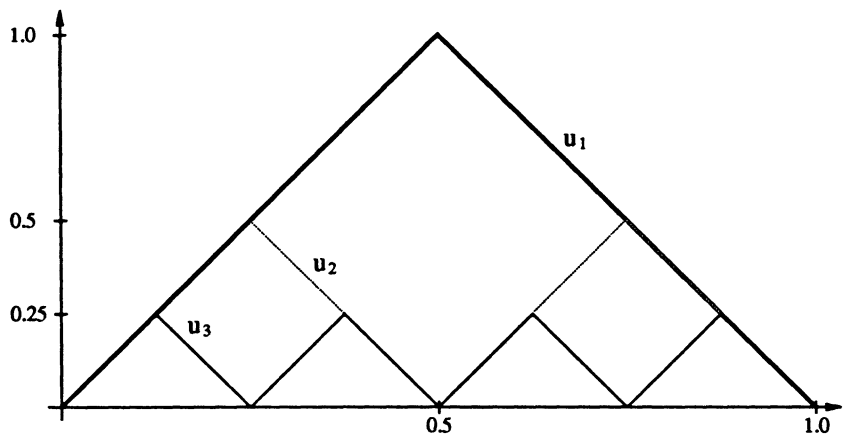
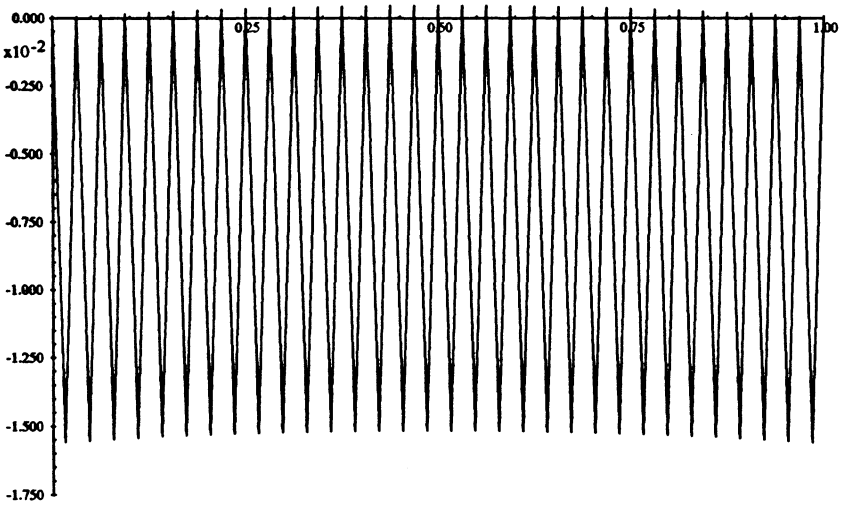
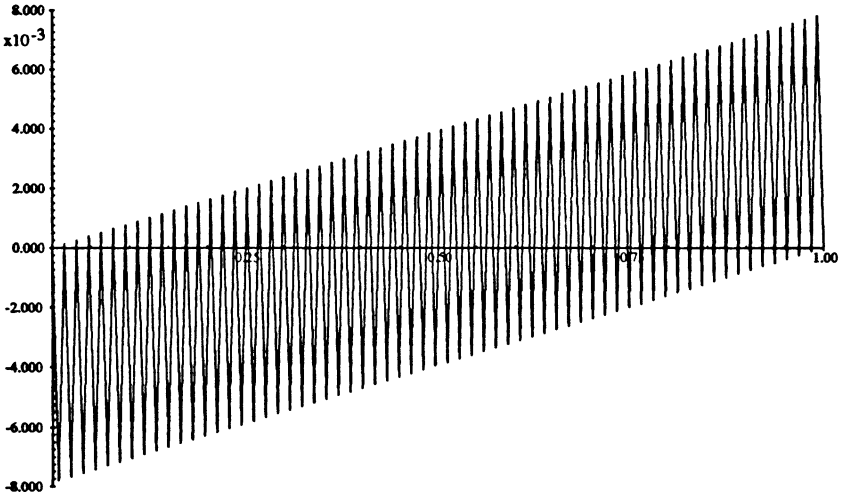


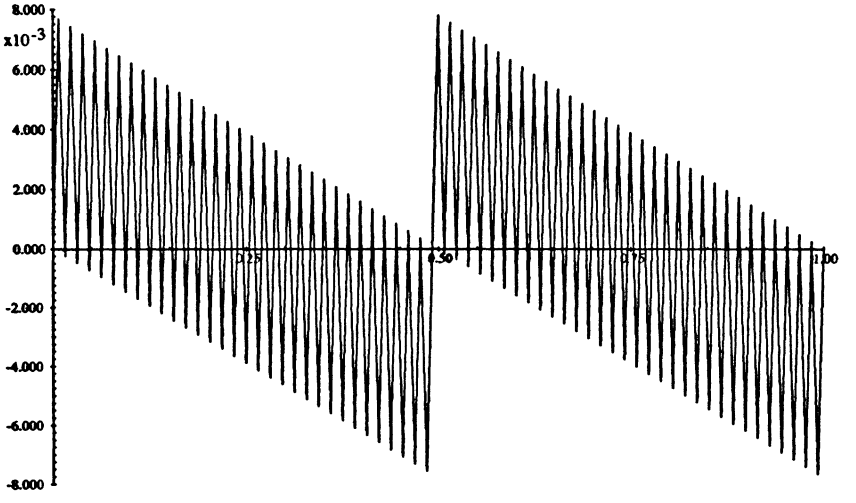
Figure 1. $W^{1,\infty}$ Local Minimizers of Young's Problem.



(a) 64 Elements.

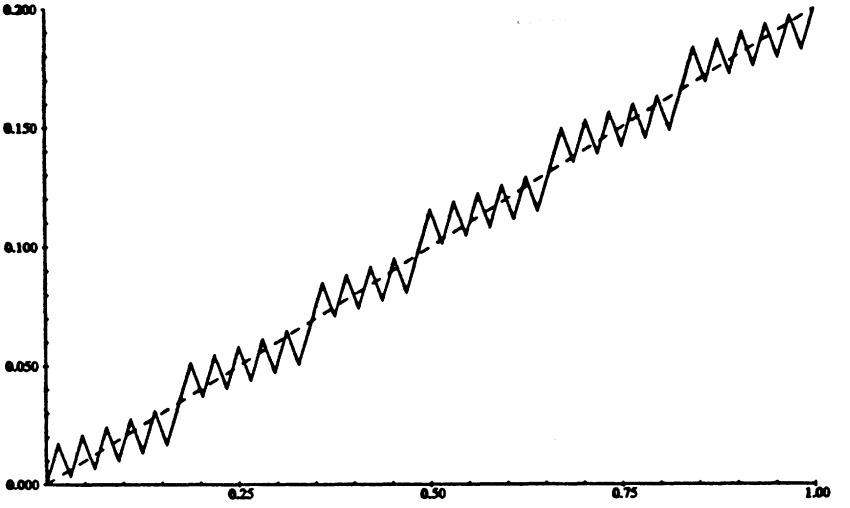


(b) 127 Elements.

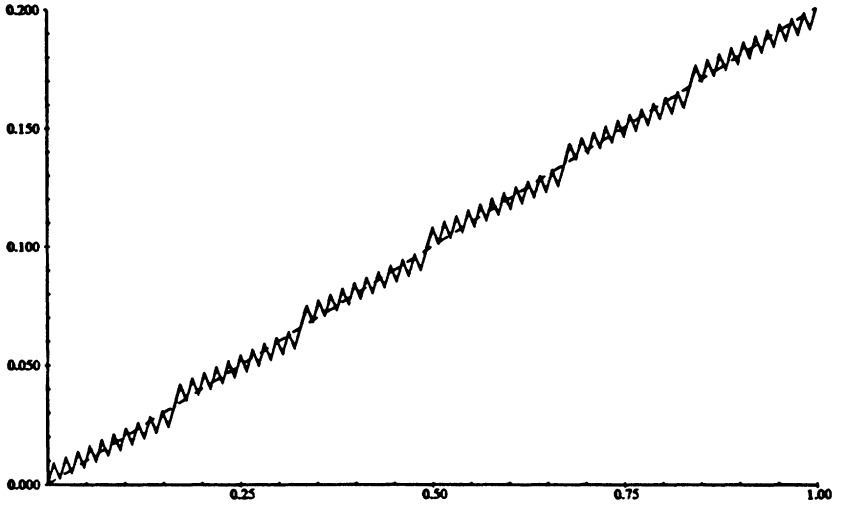


(c) 128 Elemens.

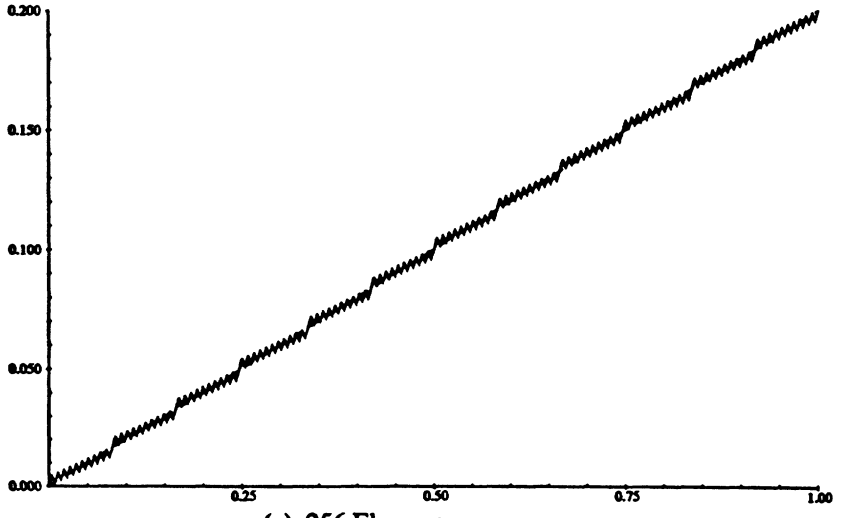
Figure 2. Young's Problem.



(a) 64 Elements.

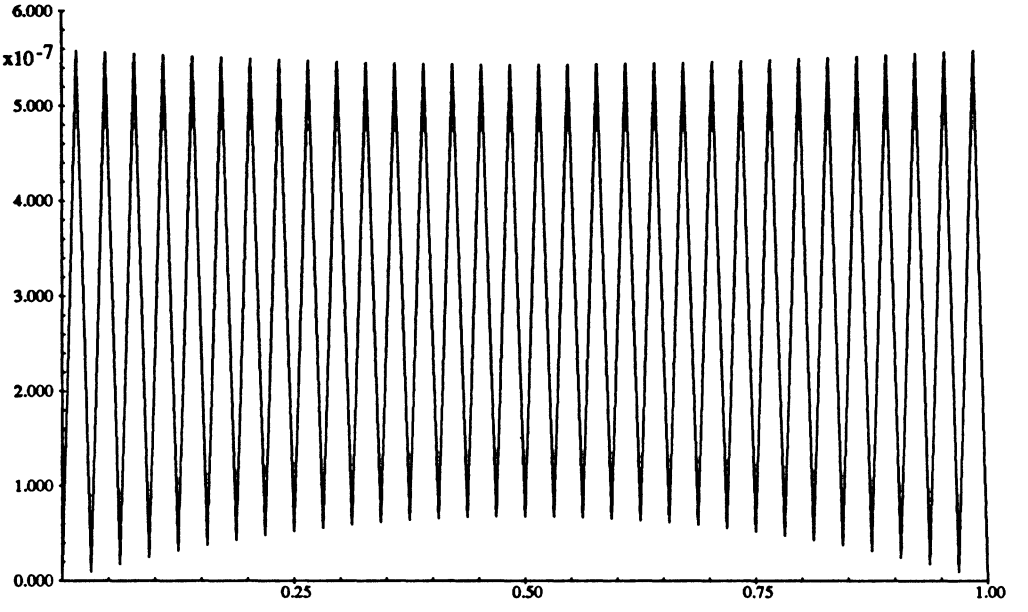


(b) 128 Elements.

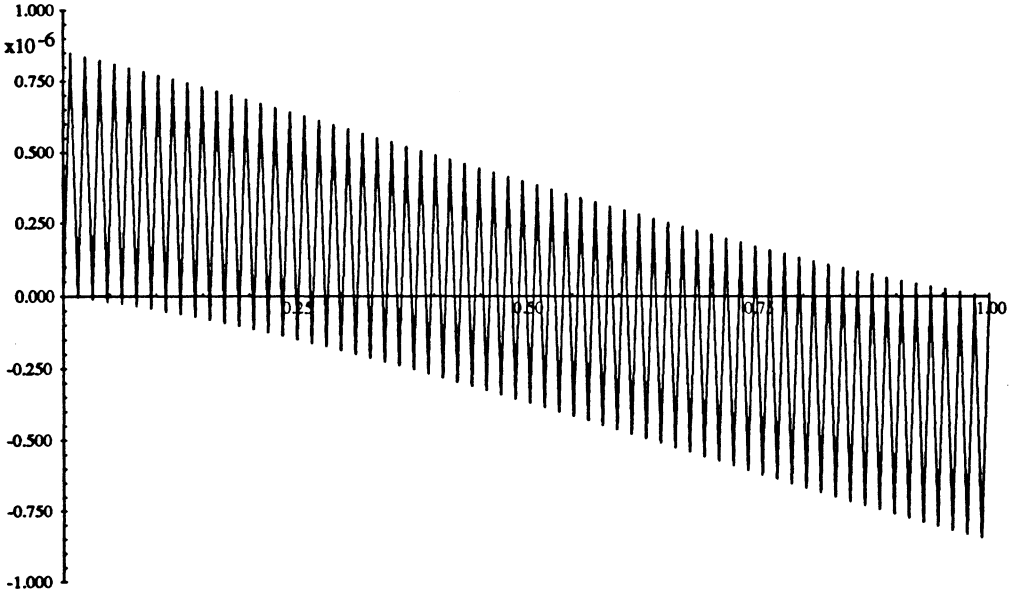


(c) 256 Elemens.

Figure 3. Non-Homogeneous Young's Problem.

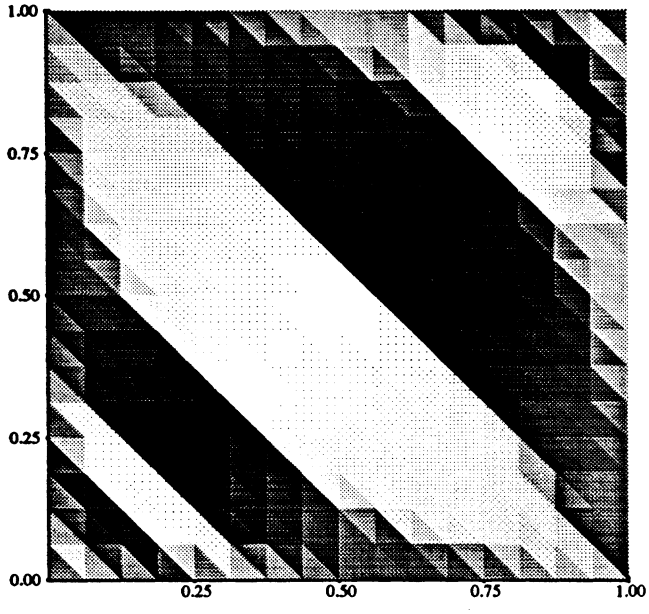


(a) 64 Elements.

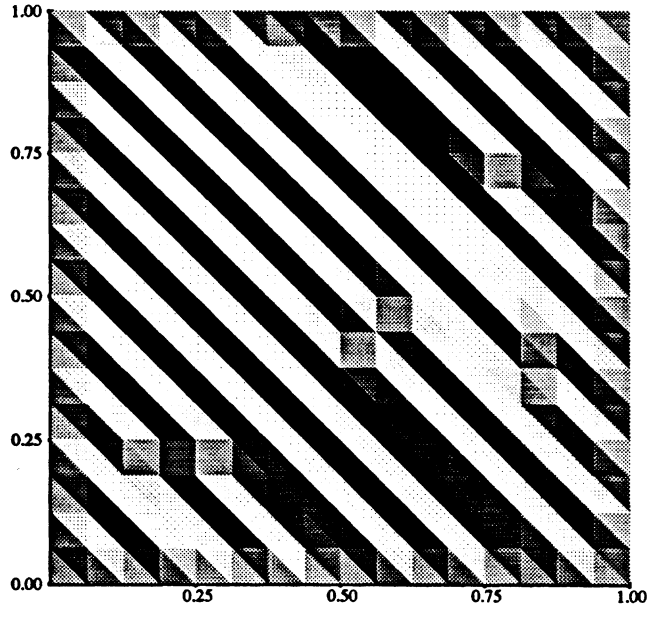


(b) 127 Elements.

Figure 4. Second Order Remainders.

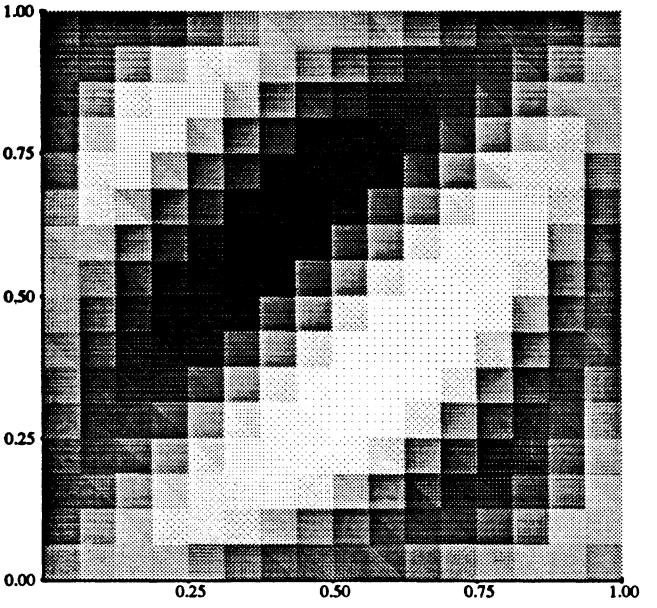


(a) Descent Algorithm, Energy = 1.4846.

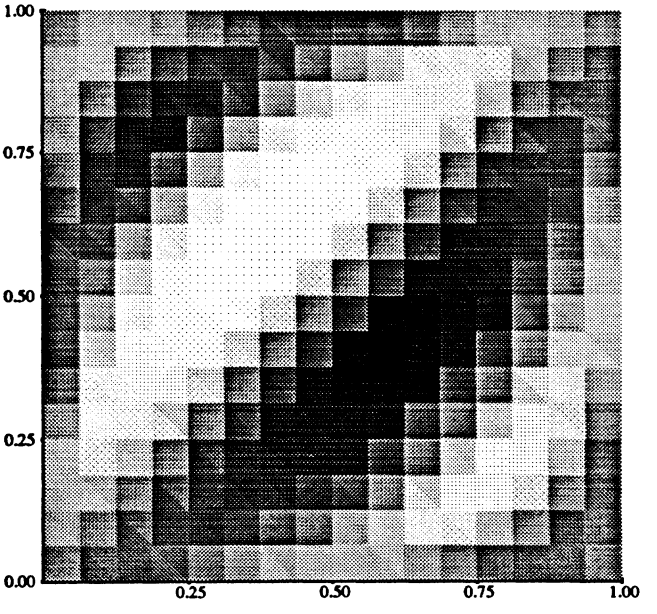


(b) Composite Algorithm, Energy = 1.0152.

Figure 7. Conforming Elements.
Black = (1,1) well, White = (-1,-1) well.



(a) Descent Algorithm, Energy = 2.6436.



(b) Composite Algorithm, Energy = 2.6436.

Figure 8. Conforming Elements.
Black = (1,-1) well, White = (-1,1) well.

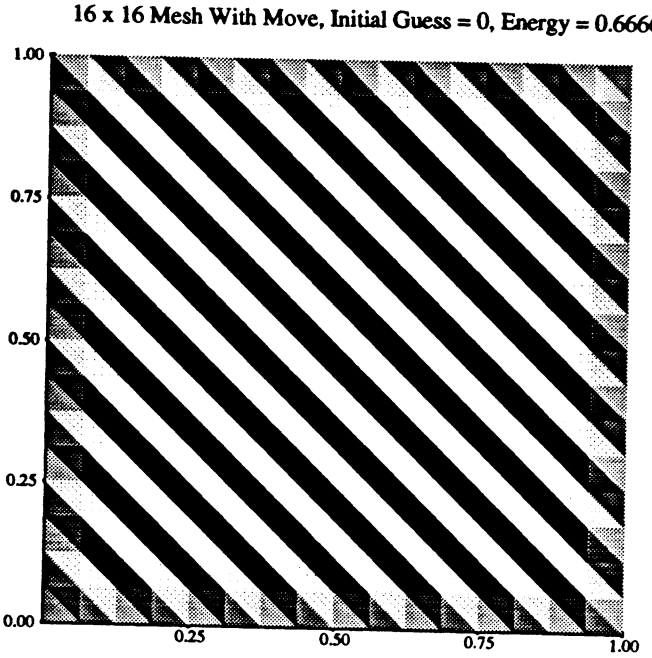
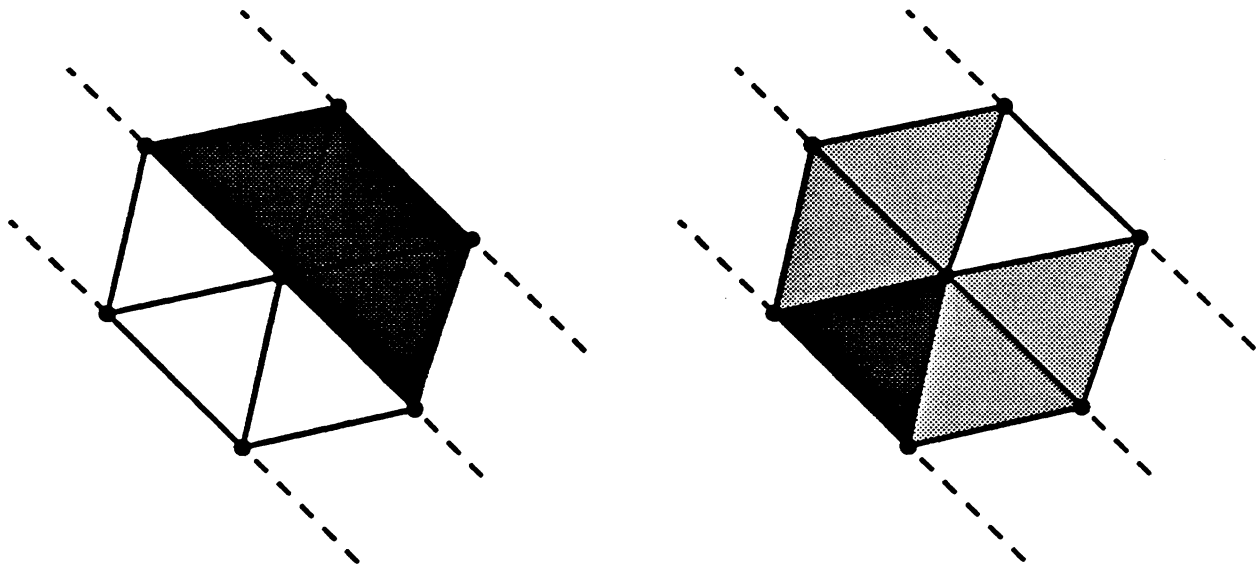
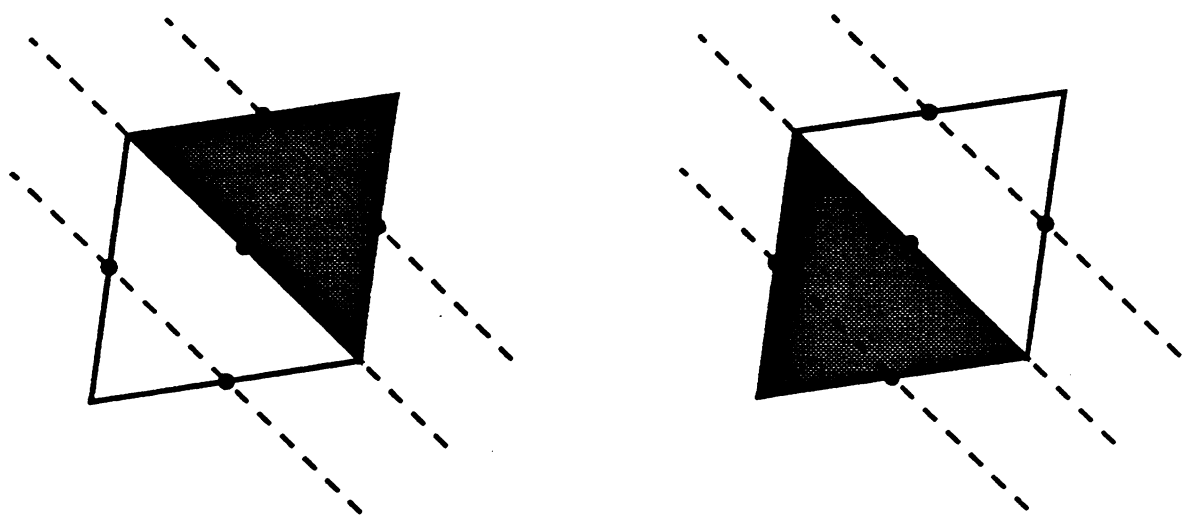


Figure 9. Conforming Elements with Zero Initial Guess.
Black = (1,1) well, White = (-1,-1) well.

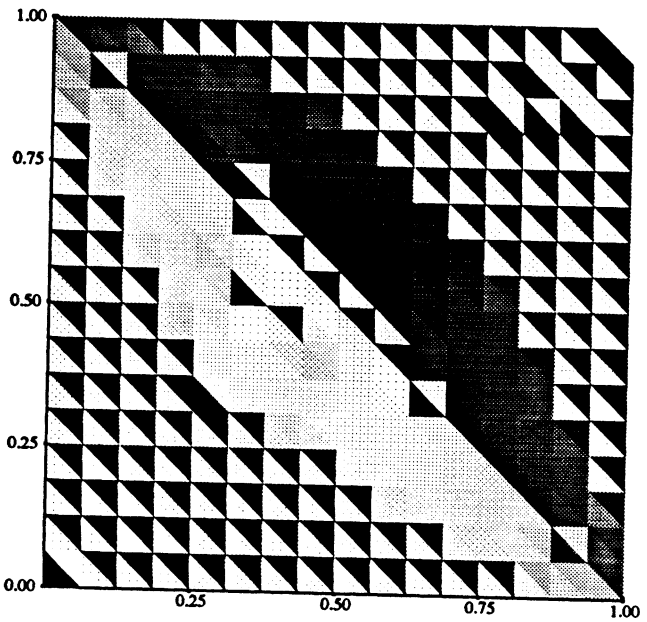


(a) Conforming Mesh.

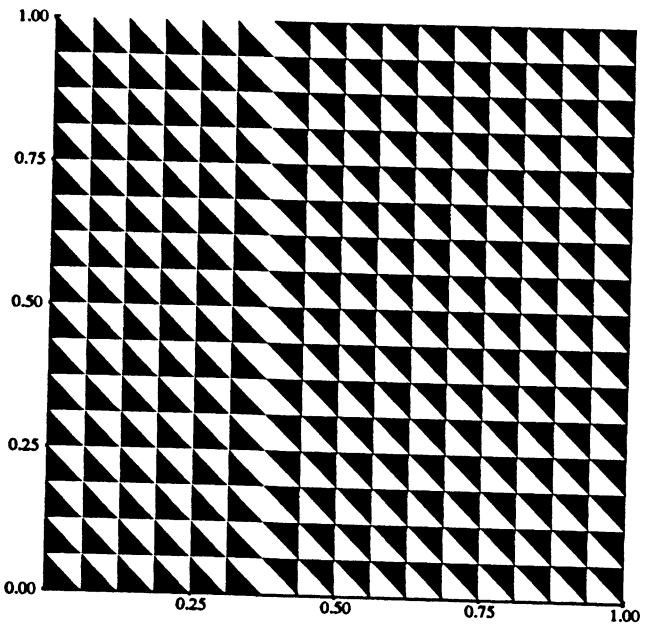


(b) Non-Conforming Mesh.

Figure 10. Adjusting Nodal Values of Different Basis Functions.

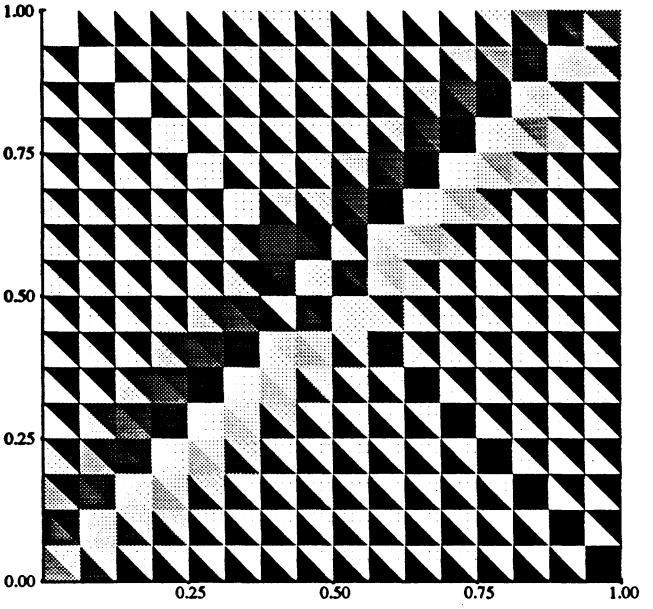


(a) Descent Algorithm, Energy = 0.5647

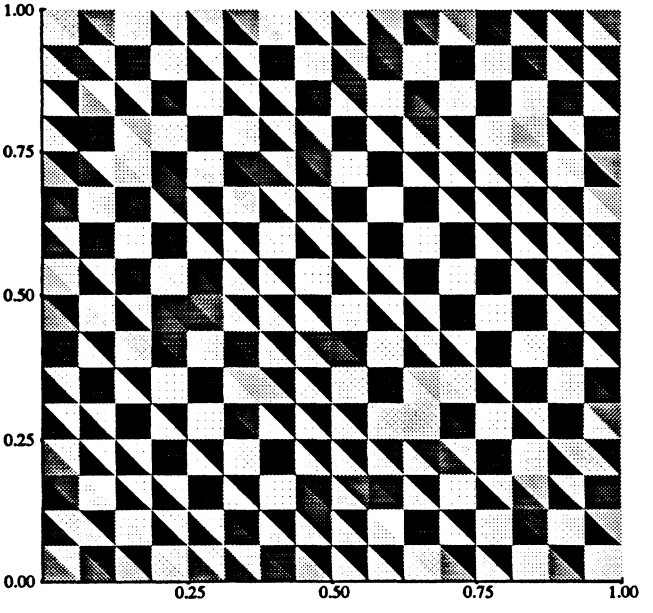


(b) Composite Algorithm, Energy = 0.000163

Figure 11. Non-Conforming Elements.
Black = (1,1) well, White = (-1,-1) well.



(a) Descent Algorithm, Energy = 0.3402



(b) Composite Algorithm, Energy = 0.5154

Figure 12. Non-Conforming Elements.
Black = (1,-1) well, White = (-1,1) well.

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